COMPUTATIONAL MECHANICS MODELLING OF CARBON NANOTUBE–BASED NANOCOMPOSITES

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To all my beloved family members;

my adorable parents, my lovely husband,

my kind sisters

and

to the new sweet member of my family, Ava.

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ABSTRACT

Composites are engineered materials that consist of two or more insoluble phases combined together; a continuous phase, known as the matrix, as well as interdispersed component known as the reinforcing phases. If at least one of the constituent phases of a composite material is less than 100 nm in size, e.g. the reinforcing phase, this composite is commonly termed nanocomposite. Among all the variety of different fillers that can be used as a nanocomposite's reinforcing phase, carbon nanotubes (CNTs), have shown to be promising candidates for their very specific and remarkable mechanical and physical properties. Carbon nanotube–based nanocomposites, i.e. composite materials in which carbon nanotubes are used as the composite's reinforcing phase, are therefore very much interesting for scientists and scholars, for the many outstanding applications that they can contribute to the world of science and industry. This study uses a computational mechanics approach to numerically characterise the properties of single– and multi–walled carbon nanotubes by simulating their molecular structure, by the finite element method, at the first stage. Special emphasis is given to investigate the effect of some imperfections in the structure of both single– and multi–walled CNTs on their mechanical properties, namely perturbation, missing atoms and silicon doping in the structure of CNTs. Later on, a unit cell of a composite material, consisting of a single CNT and its surrounding matrix is simulated and studied and finally, parallel CNTs, as reinforcement fibres in a macroscopic polymer matrix, are randomly distributed and modelled to obtain the mechanical properties of the structure and observe how random distribution of short fibres influences the properties of nanocomposites. Based on the results of this research, any type of imperfection in the structure of carbon nanotubes and carbon nanotube-based nanocomposites leads to a Young's modulus value of less than 1TPa.

ABSTRAK

Komposit adalah bahan kejuruteraan yang terdiri daripada dua atau lebih fasatidak larut yang digabungkan bersama–sama; fasa sejajar, yang dikenali sebagai matriks, serta komponen tersebar–dalam yang dikenali sebagai fasa pengukuh. Jika sekurang–kurangnya satu fasa unsur bahan komposit adalah kurang daripada 100nm dalam saiz, contohnya bagi fasa pengukuh, komposit ini biasanya diistilahkan sebagai nanokomposit.Di kalangan semua pelbagai bahan pengisi yang berbeza yang boleh digunakan sebagai fasa pengukuh, nanotuib karbon (carbon nanotubes – CNTs), telah menunjukkan kebolehannya untuk menjadi calon terbaik yang sangat khusus dan luar biasa dari sifat mekanikal dan fizikalnya. Nanokomposit berasaskan nanotiub karbon, iaitubahan komposit di mana nanotiub karbon digunakan sebagai fasa pengukuh komposit, adalah sangat menarik untuk digunakan oleh ahli–ahli sains dan cendekiawan, bagi banyak aplikasi yang boleh disumbangkan kepada dunia sains dan juga industri.Fokus utama kajian ini adalah untuk mencirikan sifat–sifat nanotiub karbon berdindingtunggal dan berdindingpelbagai dengan membuat simulasi struktur molekul mereka menggunakan kaedah unsurterhingga, pada peringkat pertama. Tumpuan khusus akan diberi untuk mengkaji kesanketidaksempurnaan dalam struktur kedua–dua CNTs berdinding tunggal dan berdindingpelbagai ke atassifat mekanikal mereka. Kemudian, sel unit bahan komposit yang terdiri daripada CNTtunggal dan matriks sekitarnya akan disimulasi dan dikaji dan akhirnya CNTs sebagai pengisi tetulang dalam matriks polimer makroskopik akan dimodelkan dan dikaji untuk mendapatkan sifat–sifat mekanik struktur.Berdasarkan keputusan kajian ini, apa-apa jenis ketidaksempurnaan dalam struktur nanotiub karbon dan nanokomposit berasakan karbon nanotiub akan mengakibatkan nilai modulus Young kurang daripada 1TPa.

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LIST OF ABBREVIATIONS

FEM	–	Finite element method
MD	–	Molecular dynamics
CNT	–	Carbon nanotube
SWCNT	–	Single–walled carbon nanotube
DWCNT	–	Double–walled carbon nanotube
MWCNT	–	Multi–walled carbon nanotubes
TEM	–	Transmission electron microscope
RM	–	Rule of mixture
HDPE	–	High density polyethylene
BEM	–	Boundary element method
RVE	–	Representative volume element
ERM	–	Effective reinforcing modulus
nano–Al	–	Nanocrystalline–aluminium
UHMWPE	–	Ultrahigh molecular weight polyethylene
PET	–	Poly ethylene terephthalate

LIST OF SYMBOLS

$\overrightarrow{C_h}$	–	Chiral vector
θ	–	Chiral angle
a_0	–	Length of each unit vector
b	–	Carbon–carbon bond length
R	–	Radius
D, d	–	Diameter
t	–	Thickness
r	–	Distance
L	–	Length
A	–	Area
$\bar{m}$	–	Mass density
V_{LJ}	–	Lennard–Jones potential
F_{LJ}	–	Lennard–Jones force
σ	–	Stress
ε	–	Strain
F	–	Force
T	–	Torque
P_{cr}	–	Critical load
f	–	Resonance frequency
E	–	Young’s modulus
G	–	Shear modulus
ν	–	Poisson’s ratio
V_{CNT}	–	Volume fraction of CNTs
U	–	Strain energy
P	–	Pure axial load

M	–	Pure bending moment
T	–	Pure twisting moment
I	–	Second moment of area
J	–	Polar moment
Δb, $\Delta\alpha$ and $\Delta\beta$	–	Tensile, bending and twist angle deformations
η_{L}	–	Length efficiency factor
η_{o}	–	Orientation efficiency factor
k_r, k_θ and k_φ	–	Molecular mechanics force constants
k	–	Spring constant
K	–	Effective length constant

CHAPTER 1

INTRODUCTION

Composites are engineered materials that consist of two or more insoluble phases combined together; a continuous phase, known as *the matrix*, as well as interdispersed components known as the *reinforcing phase*. The matrix is typically the major constituent that provides durability for the overall composite and it can be for instance, a metallic, a ceramic or a polymer material. The reinforcing inclusions are the structure's load carriers that can be in the form of fibres, particles, or flakes. This phase of the composite structure provides its stiffness and strength. Now if at least one of the constituent phases of a composite material is less than 100 nm in size, e.g. the reinforcing phase, this composite is commonly termed *nanocomposite*.

1.1 Composite structure

The reinforcing phase and matrix are the major constituents in all reinforced polymer composites. Therefore, suitable selection of type, amount and orientation of these components is very important and has a significant effect on the characteristics of the produced composite; such as its tensile and compressive strengths, fatigue strength and failure mechanisms, electrical and thermal conductivities, specific gravity, and cost (Kaw, 2006).

1.1.1 Reinforcing phase types

Fibres can be classified as follows:

(a) Glass fibres

Glass fibres are usually isotropic and as a result of their low cost, high chemical resistance, excellent insulating properties and high tensile strength, they are the most common reinforcing materials for polymeric matrix composites. However, they have some disadvantages such as low tensile modulus, relatively high specific gravity, low fatigue resistance, high hardness and sensitivity to abrasion that decrease their tensile strength. The two most important kinds of glass fibres are called *E–glass* fibres, named because of their high electrical properties, and *S–glass* fibres, named so because of their high tensile strength (Kaw, 2006).

(b) Aramid fibres

These types of fibres are anisotropic and the most widely used *organic* fibres. Tensile strength, stiffness, and toughness of them are very high in the axial direction of the fibre. However, their tensile strength and stiffness in the transverse direction is relatively low. Low compressive strength is the major disadvantage of these types of reinforcing fibres.

(c) Boron fibres

Boron fibres are one of the first high performance fibres available for use as reinforcing phase in composite materials. The diameter of boron fibres is in the range of 0.1–0.2 mm, which is an order of magnitude larger than glass, aramids, or graphite fibres. But their large diameter and high stiffness restricts their bend radius greatly, offering high resistance to buckling, which in turn contribute to an excellent compressive performance of boron–reinforced composites.

(d) Ceramic fibres

Some examples of ceramic fibres are *silicon carbide* and *aluminium–boron–silica* fibres. An outstanding feature offered by ceramic fibres is their resistance to extremely high temperatures, while still maintaining competitive structural properties. Having applications in metal and ceramic matrix composites, ceramic fibres are suitable options for reinforcing metal matrices in which boron and carbon fibres exhibit adverse reactivities.

(e) Graphite and carbon fibres

The terms *graphite* and *carbon* are often interchangeably used in the composite community. Major advantages of carbon fibres are their extraordinarily high tensile strength–weight ratios, as well as tensile modulus–weight ratios, very low coefficient of thermal expansion and high fatigue strengths. They behave anisotropic and have a high longitudinal stiffness due to alignment of the basal planes parallel to the fibre axis. Their low impact resistance and high cost are their major disadvantages, but these reinforcing materials are mostly very appropriate options in aerospace industry, where weight savings is considered to be more critical than lowering costs.

Transferring stresses between the fibres and protect the surface of the fibres from mechanical abrasion are the main role of the matrix in a fibre–reinforced composite. The matrix provides lateral support against the possibility of fibre buckling under compression loading (Kaw, 2006).

1.1.2 Matrix phase types

Matrices can be classified as follows:

(a) Polymeric matrix

Polymer is defined as a long chain of molecules, containing one or more repeating units of atoms joined together by strong covalent bonds. Polymeric materials are collections of a large number of polymer molecules of similar chemical structure, but not necessarily of equal length. In solid state, these molecules are either frozen in space in a random fashion, e.g. for amorphous polymers, or in a mixture of random and orderly folded fashions, e.g. for semi–crystalline polymers.

Among different types of polymeric matrices, thermoplastic and thermoset polymer matrices are two major categories. In thermoplastic polymers, individual molecules are linear in structure, without any chemical linking between them. Thermoset polymers, on the other hand, consist of molecules which are chemically joined together by cross–links, forming a rigid three–dimensional network structure during polymerization reaction which as a result, cannot be easily melted or reshaped under heat and pressure.

(b) Metal matrix

Metals have high modulus and yield strength which candidate them for applications requiring high transverse strength and compressive strength. Another important advantage of a metal matrix, over the polymeric matrix, is its long–term resistance to severe environmental conditions, such as being used in high temperatures, or enduring a variety of mechanical and thermal treatments, allowing them to be plastically deformed and strengthened.

Metals have some disadvantages as well, such as high specific weight, high melting points and hence hard to process. They also have the tendency toward corrosion at the matrix/fibre interface (Kaw, 2006).

1.1.3 Carbon nanotube–based composites

Among all the variety of different fillers that can be used as a nanocomposite's reinforcing phase, *carbon nanotubes* (CNTs), have shown to be promising candidates for their very specific mechanical and physical properties which will be explained later. carbon nanotube–based nanocomposites, i.e. composite materials in which carbon nanotubes are used as the composite's reinforcing phase, are therefore very much interesting for scientists and scholars, for the many outstanding and remarkable applications that they can contribute to the world of science and industry. They are expected to influence many fields in terms of technology and industry. They will have applications in many diverse fields such as energy, signal processing, medicine, biotechnology, information technology, aerospace, agriculture, and environment (Wang *et al.*, 2010). These outstanding materials can be used as stand–alone nanomaterials or as reinforcements in composites for a wide variety of application. Therefore, several detailed studies have been conducted to explore different properties of carbon nanotubes and carbon nanotube based composite materials.

Composite materials mostly show more significant advantageous properties compared to monolithic materials. Monolithic metals and their alloys cannot always meet the demands of today's advanced technologies and performance requirements. It means that by incorporating reinforcements into a, for instance, metallic, ceramic or polymer matrix, the properties of the matrix improves to a higher mechanical strength, more significant temperature stability and better chemical durability. The existence of reinforcing elements improves the structure's physical and chemical properties.

The main focus of the project is therefore to characterise the properties of single– and multi–walled carbon nanotubes by simulating their molecular structure using the *finite element method* (FEM), at the first stage. Special emphasis will be given to investigate the effect of *imperfections* in the structure of both single– and multi–walled CNTs on their mechanical properties. Later on, a unit cell of a composite material consisting of a single CNT and its surrounding matrix will be simulated and studied and finally CNTs as reinforcement fillers in a macroscopic polymer matrix will be modelled and studied to obtain the mechanical properties of the structure.

1.2 Statement of problem

There are very vast variety of emerging applications for CNTs and CNT–based polymer nanocomposites, ranging from nano–electronics to biomedical devices. Due to the restrictions in manufacturing perfect CNTs, different configurations of defects in CNTs should be investigated before proceeding to the high cost of making them experimentally available; namely, *vacancies* i.e. single or several carbon atoms being missed in the related C–C bonds and therefore in the whole structure, improper location of carbon atoms making the structure *perturbated*, as well as the existence of other atoms *doped* in the structure that will all influence the properties of nanostructure material.

Finding out *how defects and imperfections influence the mechanical properties of different types of CNTs and CNT–based polymer nanocomposites,* before getting involved in the burden of experimental production and its pertinent high expenses is the main issue that this investigation tries to study as much as possible. It is quite necessary and helpful to study how these defects and imperfections influence the mechanical properties of different types of CNTs and to embed them later in a polymer matrix and study the properties of the nanocomposite for its potential applications ranging from nanoelectronics to biomedical devices.

1.3 Scopes of the study

(a) To characterise the properties of single– and multi–walled carbon nanotubes by simulating their molecular structure using the finite element method.

(b) To model and study the composite material consisting of CNTs as reinforcement fillers inside a polymer matrix.

(c) Special emphasis will be given to investigate the effect of imperfections in the structure of both single–and multi–walled CNTs as nanocomposites' reinforcement elements independently, as well as the randomness of the distribution of fibres inside matrix, on the mechanical and physical properties of the whole structure by means of the finite element method.

1.4 Research objectives

The objectives of this research can be stated as follows:

(a) To determine the effects of deficiencies and imperfections in carbon nanotube's structure on its main mechanical properties.

(b) To simulate the structure of a unit cells of CNT/polymer matrix nanostructure as a basic investigation for evaluating the macroscopic structure later.

(c) To simulate the macroscopic structure of different CNT/polymer matrices and study their mechanical and physical properties with different orientations and dispersion densities.

1.5 Structure of the thesis

This dissertation is organised in five chapters as follows:

Chapter 1, the current chapter, looks mainly on the significance of the research topic and gives a general definition of nanocomposites and carbon nanotube–based composites. The scopes and objectives of the research are also presented in this chapter.

Chapter 2 is arranged to introduce the basic definitions pertaining to the involved nanomaterials and to give a brief review of the main steps forward in the path of characterising the above–mentioned nanostructures.

The methods applied and the steps taken for investigating the structures' properties and achieving the appropriate results are presented in *Chapter 3*, whereas the obtained results are depicted and discussed in detail in *Chapter 4*.

Finally, a conclusion of the whole research approach and the achieved results is introduced in *Chapter 5*.

REFERENCES

Aboudi J. (1991). *Mechanics of composite materials: a unified micromechanical approach* (*Studies in Applied Mechanics*). ElsevierScience Ltd.

Ajayan P. M., Ebbesen T. W., Ichihashi T., Iijima S., Tanigaki K., and Hiura H. (1993). Opening carbon nanotubes with oxygen and implications of filling. *Nature* 362, 522–525.

Ajayan P. M., and Iijima S. (1993). Capillarity–induced filling of carbon nanotubes. *Nature* 361, 333–334.

Ajayan P. M., Stephan O., Colliex C., and Trauth D. (1994). Aligned carbon nanotube arrays formed by cutting a polymer resin nanotube composite. *Science* 265, 1212–1214.

Ajayan P. M. (1999). Nanotubes from carbon. *Chem. Rev.* 99, 1787–1799.

Baibarac M., and Gomez–Romero P. (2006). Nanocomposites based on conducting polymers and carbon nanotubes: From fancy materials to functional applications. *J. Nansci. Nanotechnol.* 6, 289–302.

Baughman R. H., Zakhidov A. A., and De Heer W. A. (2002). Carbon nanotubes–the route toward application. *Science* 197, 787–792.

Bethune D. S., Kiang C. H., De Vries M. S., Gorman G., Savoy R., Vazquez J., and Beyers R. (1993). Cobalt–catalysed growth of carbon nanotubes with single–atomic–layer walls. *Nature* 363, 605–607.

Benveniste Y. (1987). A new approach to the application of Mori–Tanaka's theory in composite materials. *Mech. Mater.*6, 147–157.

Bianco A., Kostarelos K., Partidos C. D., and Prato M. (2005). Biomedical applications of functionalised carbon nanotubes. *Chem. Commun.* 5, 571–577.

Bubert H., Haiber S., Brandl W., Marginean G., Heintze M., and Bruse V. (2003). Characterization of the uppermost layer of plasma–treated carbon nanotubes. *Diamond Relat. Mater.* 12, 811–815.

Chang T., and Gao H. (2003). Size–dependent elastic properties of single–walled carbon nanotubes via a molecular mechanics model. *J. Mech. Phys. Solids* 51, 1059–1074.

Chen X. L., and Liu Y. J. (2004). Square representative volume elements forevaluating the effective material properties of carbon nanotube–basedcomposites. *Comp. Mater. Sci.* 29, 1–11.

Chiang C. R. (1994). A statistical theory of the tensile strength of short–fibre–reinforced composites. *Compos. Sci. Technol.* 50, 479–482.

Cho W. S. To (2006). Bending and shear moduli of single–walled carbon nanotubes. *Finite Elem. Anal. Des.* 42,404–413.

Coleman J. N., Khan U., Blau W. J., and Gun'ko Y. K. (2006). Small but strong–a review of the mechanical properties of carbon nanotube–polymer composites. *Carbon* 44, 1624–1652.

Cordero B., Gómez V., Platero–Prats A. E., Revés M., Echeverría J., Cremades E., BarragánandF., and Alvarez S. (2008) Covalent radii revisited. *Dalton Trans* 21, 2832–2838.

Cox H. L. (1952). The elasticity and strength of paper and other fibrous materials. *Brit. J. Appl. Phys.* 3, 72–79.

Dai L., and Mau A. W. H. (2001). Controlled synthesis and modification of carbon nanotubes and C60: Carbon nanostructures for advanced polymeric composite materials. *Adv. Mater.* 13, 899–913.

De Los Santos H. J. (1999). *Introduction to microelectromechanical microwave systems*. London : Artech House Publishers.

Dresselhaus M. S., Dresselhaus G., and Saito R. (1995). Physics of carbon nanotubes. *Carbon* 33, 883–891.

Dresselhaus M. S., Dresselhaus G., and Eklund P. (1996). *Science of fullerenes and carbon nanotubes*. New York: Academic Press.

Dresselhaus M. S., Dresselhaus G., and Avouris Ph. (2001). *Carbon nanotubes synthesis, structure, properties and applications*. Berlin: Springer–Verlag.

Edidin A. A., and Kurtz S. M. (2001). Development and validation of the small punch test for UHMWPE used in total joint replacements. *Key Eng. Mater.* 198, 1–40.

Esawi A. M. K., and Farag M. M. (2007). Carbon nanotubes reinforced composites: Potential and current challenges. *Mater. Design* 28, 2394–2401.

Eslami Afrooz I., Öchsner A., and Rahmandoust M. (2012). Effects of the carbon nanotube distribution on the macroscopic stiffness of composite materials. *Comp. Mater. Sci.* 51, 422–429.

Fan C. W., Liu Y. Y., and Hwu C. (2009). Finite element simulation for estimating the mechanical properties of multi–walled carbon nanotubes. *Appl. Phys. A* 95, 819–831.

Fereidoon A., Saeedi E., and Ahmadimoghadam B. (2008). *Comparison between different finite element methods for foreseeing the elastic properties of carbon nanotube reinforced epoxy resin composite*. London: Proceedings of the World Congress on Engineering 2008 (WCE2008) Vol II.

Ferrari M., and Johnson G. C. (1989). The effective elasticities of short fibre composites with arbitrary orientation distribution. *Mech. Mater*. 8, 67–73.

Fisher F. T., Bradshaw R. D., and Brinson L. C. (2003). Fibre waviness in nanotube–reinforced polymer composites–I: modulus predictions using effective nanotube properties. *Compos. Sci. Technol.* 63, 1689–1703.

Fukuda H., and Kawata K. (1974). On young's modulus of short fibre composites. *Fibre Sci. Technol.* 7, 207–222.

Gal'pern E. G., Stankevich I. V., Chistyakov A. L., and Chernozatonskii L. A. (1992). Atomic and electronic structure of the barrelenes b–$C_m$with m=36+12n. *JETP Lett.* 55, 483–486.

Gómez–del Rio T., Poza P., Rodriguez J., Garcia–Gutierrez M. C., Hernandez J. J., and Ezquerra T. A. (2010). Influence of single–walled carbon nanotubes on the effective elastic constants of poly (ethylene terephthalate). *Compos. Sci. Technol.* 70, 284–290.

Goze C., Bernier P., Henrard L., Vaccarini L., Hernandez E., and Rubio A. (1999). Elastic and mechanical properties of carbon nanotubes. *Synthetic Met.* 103, 2500–2501.

Halpin J. C., and Kardos J. L. (1976). The Halpin–Tsai equations: A review. *Polym. Eng. Sci.* 16, 344–352.

Hashin Z. (1983). Analysis of composite materials. *J. Appl. Mech*. 50, 481–506.

Hill R. (1963). Elastic properties of reinforced solids: some theoretical principles. *J. Mech. Phys. Solids* 11, 357–372.

Iijima S. (1991). Helical microtubules of graphitic carbon. *Nature* 354, 56–58.

Iijima S., and Ichihashi T. (1993). Single–shell carbon nanotubes of 1–nm diameter. *Nature* 363, 603–605.

Iijima S. (2002). Carbon nanotubes: Past, present, and future. *Physica B* 323, 1–5.

Irvine T. (1999). *Application of the Newton–Raphson method to vibration problems*. Vibration data Publications.

Jin Y., and Yuan F. G. (2003). Simulation of elastic properties of single–walled carbon nanotubes. *Compos. Sci. Technol.* 63, 1507–1515.

Kalamkarov A. L., Georgiades A. V., Rokkam S. K., Veedu V. P., and Ghasemi–Nejhad M. N. (2006). Analytical and numerical techniques to predict carbon nanotube properties. *Int. J. Solids Struct.* 43, 6832–6854.

Kalamkarov A. L., Askari D., Veedu V. P., and Ghasemi–Nejhad M. N. (2007). Generally cylindrical orthotropic constitutive properties modeling of matrix–filled single–walled nanotubes: Axial mechanical properties, *J. Compos. Mater.* 41, 757–779.

Kanagaraj S., Varanda F. R., Zhil'tsova T. V., Oliveira M. S. A., and Simões J. A. O. (2007). Mechanical properties of high density polyethylene/carbon nanotube composites. *Compos. Sci. Technol.* 67, 3071–3077.

Kanagaraj S. (2009). *CNT/polymer composites for biomedical applications*. Department of Mechanical Engineering, Indian Institute of Technology Guwahati, India.

Kosakovskaya Z. Y., Chernozatonskii L. A., and Fedorov E. A. (1992). Nanofilament carbon structure. *JETP Lett.* 56, 26–29.

Krenchel H. (1964). *Fibre reinforcement–theoretical and practical investigations of the elasticity and strength of fibre–reinforced materials*. Copenhagen : Akademisk Forlag.

Krishnan A., Dujardin E., Ebbesen T. W., Yianilos P. N., and Tracy M. M. J. (1998). Young's modulus of single–walled carbon nanotubes, *Phys. Rev. B*58, 14013–14019.

Kurtz S. M., Foulds J. R., Jewett C. W., Srivastav S., and Edidin A. A. (1997). Validation of a small punch testing technique to characterize the mechanical behaviour of ultra–high–molecular–polyethylene. *Biomaterials* 18, 1659–1663.

Lau K. T., and Hui D. (2002). Effectiveness of using carbon nanotubes as nano–reinforcements for advanced composite structures. *Carbon* 40, 1605–1606.

Li C., and Chou T. W. (2003). A structural mechanics approach for the analysis of carbon nanotubes. *Int. J. Solids Struct.* 40, 2487–2499.

Liang C., Shimizu Y., Sasaki T., Umehara H., and Koshizaki N. (2004). One–step growth of silica nanotubes and simultaneous filling with indium sulfide nanorods. *J. Mater. Chem.* 14, 248–252.

Liu Y. J., and Chen X. L. (2003) (I). Continuum models of carbon nanotube–based composites using the boundary element method. *Electron. J. Bound. Elem*. 1, 316–335.

Liu Y. J., and Chen X. L. (2003) (II). Evaluations of the effective material properties of carbon nanotube–based composites using a nanoscale representative volume element. *Mech. Mater*. 35, 69–81.

Liu Y., NishimuraN., and Otani Y. (2005). Large–scale modeling of carbon–nanotube composites by a fast multipole boundary element method. *Comp. Mater. Sci.* 34, 173–187.

Lu J. P. (1997). Elastic properties of carbon nanotubes and nanoropes. *Phys. Rev. Lett.* 79, 1297–1300.

Mavalizadeh S. M., Rahmandoust M., and Öchsner A. (2011). Numerical investigation of the overall stiffness of carbon nanotube based composite materials. *J. Nano Res.* 13, 47–59.

McLaughlin R. (1977). A study of the differential scheme for composites materials. *Int. J. Eng. Sci*. 15, 237–244.

Mora R. J., Vilatela J. J., and Windle A.H. (2009). Properties of composites of carbon nanotube fibres. *Compos. Sci. Technol.* 69, 1558–1563.

Mori T., and Tanaka, K. (1973). Average stress in the matrix and average elastic energy of materials with misfitting inclusions. *Acta metall.* 21, 571–574

Mura T. (1987). *Micromechanics of defects in solids*, 2nd ed. Martinus Nijhoff Publisher.

Natsuki T., Kriengkamol T., and Morinobu E. (2004). Prediction of elastic properties for single–walled carbon nanotubes. *Carbon* 42, 39–45.

Odegard G. M., Gates T. S., Nicholson L. M., and Wise K. E. (2001). Equivalent continuum modelling of nano–structured materials. *NASA TM* 62, 1869–1880.

Pipes R. B., and Hubert P. (2002). Helical carbon nanotube arrays: Mechanical properties. *Compos. Sci. Technol.* 62, 419–428.

Rahmandoust M., and Öchsner A. (2009). Influence of structural imperfections and doping on the mechanical properties of single–walled carbon nanotubes. *J. Nano Res.* 6, 185–196.

Rahmandoust M., and Öchsner A. (2011). Buckling behaviour and natural frequency of zigzag and armchair single–walled carbon nanotubes. *J. Nano Res.* 16,153–160.

Rahmandoust M., and Öchsner A. (2012). On finite element modeling of single and multi–walled carbon nanotubes. *J. Nanosci. Nanotech.* 12, in press.

Shokrieh M. M., and Rafiee R. (2010). Investigation of nanotube length effect on the reinforcement efficiency in carbon nanotube based composites. *Compos. Struct.* 92, 2415–2420.

Sie C. T. (2009), *Carbon nanotube reinforced composites: Metal and ceramic matrices*. Weinheim: Wiley–VCH.

Sinnott S. B., Ni B., Mikulski P. T., and Harrison J. A. (2004). *Compression of filled carbon nanotubes: Predictions from molecular dynamics simulations*. Ninth Foresight Conference on Molecular Nanotechnology Proceeding.

Song H. Y., Sun H. M., and Zhang G. X. (2006). Molecular dynamic study of effects of Si–doping upon structure and mechanical properties of carbon nanotubes. *Commun. Theor. Phys.* 45, 741–744.

Song Y. S., and Youn J. R. (2006). Modeling of effective elastic properties for polymer based carbon nanotube composites. *Polym. Int.* 47, 1741–1748.

Tandon G. P., and Weng G. J. (1986). Average stress in the matrix and effective moduli of randomly oriented composites. *Compos. Sci. Technol.* 27, 111–132.

Tang W., Santare M. H., and Advani S. G. (2003). Melt processing and mechanical property characterization of multi–walled carbon nanotube/high density polyethylene (MWNT/HDPE) composite films. *Carbon* 41, 2779–2785.

Thostenson E. T., Ren Z., and Chou T. W. (2001). Advances in the science and technology of carbon nanotubes and their composites: A review. *Compos. Sci. Technol.* 61, 1899–1912.

Thostenson E. T., and Chou T. W. (2003),On the elastic properties of carbon nanotube–based composites: modeling and characterization. *J. Phys. D: Appl. Phys.* 36, 573–582.

Tirupathi R. C., and Ashok D. B. (1997). *Introduction to finite elements in engineering*, 2nded., New Jersey: Prentice–Hall.

Tserpes K. I., and Papanikos P. (2005). Finite element modelling of single–walled carbon nanotubes. *Compos. Part B–Eng.* 36, 468–477.

Tucker C. L., and Liang E. (1999). Stiffness predictions for unidirectional short fibre composites: Review and evaluation. *Compos. Sci. Technol.* 59, 655–671.

Wang C. M., Zhang Y. Y., Xiang Y., and Reddy J. N. (2010). Recent studies on buckling of carbon nanotubes. *Appl. Mech. Rev.* 63, 030804–1–18.

Wang H., and Yao Z. (2007). Large scale analysis of mechanical properties in 3–D fibre–reinforced composites using a new fast multipole boundary element method. *Tsinghua Sci. Technol.* 12, 554–561

Wagner H., Lourie O., Feldman Y., and Tenne R. (1998). Stress–induced fragmentation of multiwall carbon nanotubes in a polymer matrix. *Appl. Phys. Lett.* 72, 188–190.

Wu Y., Zhang X., Leung A. Y. T., and Zhong W. (2006). An energy–equivalent model on studying the mechanical properties of single–walled carbon nanotubes. *Thin Wall Struct*. 44, 667–676.

Xie S., Li W., Pan Z., Chang B., and Sun L. (2000). Mechanical and physical properties of carbon nanotube. *J. Phys. Chem. Solids* 61, 1153–1158.

Xie X. L., Mai Y. W., and Zhou X. P. (2005). Dispersion and alignment of carbon nanotubes in polymer matrix: A review. *Mater. Sci. Eng. R.* 49, 89–112.

Yu W., Xi W. X., and Xianggui N. (2004). Atomistic simulation of the torsion deformation of carbon nanotubes. *Modelling Simul. Mater. Sci. Eng.* 12, 1099–1107.

Zhu L., and Nart K. A. (2004). Numerical simulation of the effect of nanotube orientation on tensile modulus of carbon–nanotube–reinforced polymer composites. *Polym. Int.* 53, 1461–1466.

Zhong R., Cong H., and Hou P. (2002). Fabrication of nano–Al based composites reinforced by single walled carbon nanotubes, *Carbon* 41, 848–851.

Zoo Y. S., An J. W., Lim D. P., and Lim D. S. (2004). Effect of carbon nanotubes addition on tribological behaviour of UHMWPE. *Tribol. Lett.* 16, 305–309.